

chain nodes : 6 7 8 9 10 11 13 18 19 20 23

ring nodes :

1 2 3 4 5

ring/c

12

chain bonds : . .

1-7 2-6

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm b

1-2 1-5 1-7

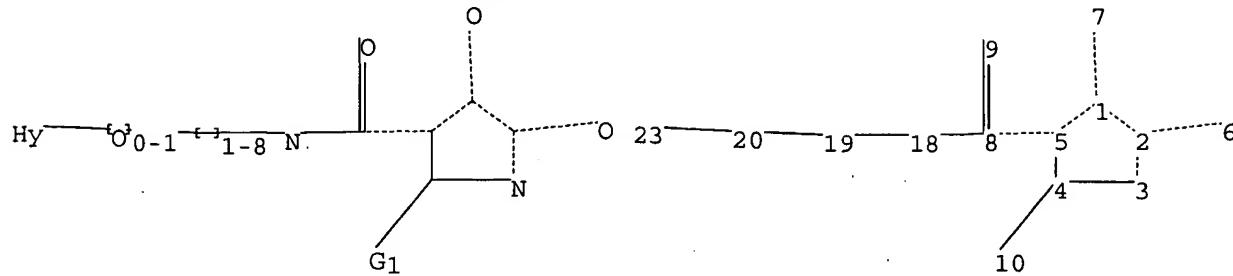
G1: [*1], [*2], [*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom 18:CLASS 19:Atom 20:CLASS 23:Atom

10/616031

=>
Uploading C:\Program Files\Stnexp\Queries\10616031-2.str



H¹

1¹

C²

1²

H³

1³

chain nodes :
6 7 8 9 10 11 13 18 19 20 23
ring nodes :
1 2 3 4 5
ring/chain nodes :
12
chain bonds :
1-7 2-6 4-10 5-8 8-9 8-18 18-19 19-20 20-23
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-7 2-3 2-6 3-4 4-5 4-10 5-8 8-9 8-18 18-19 19-20 20-23

G1: [*1], [*2], [*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:Atom 18:CLASS 19:Atom 20:CLASS 23:Atom

10/616031

chain nodes :
6 7 8 9 10 11 13 18 19 20 23
ring nodes :
1 2 3 4 5
ring/chain nodes :
12
chain bonds :
1-7 2-6 4-10 5-8 8-9 8-18 18-19 19-20 20-23
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-7 2-3 2-6 3-4 4-5 4-10 5-8 8-9 8-18 18-19 19-20 20-23

G1:[*1],[*2],[*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:Atom 18:CLASS 19:Atom 20:CLASS 23:Atom

L8 STRUCTURE UPLOADED

=> d 18
L8 HAS NO ANSWERS
L8 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 18
SAMPLE SEARCH INITIATED 18:01:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 58 TO ITERATE

100.0% PROCESSED 58 ITERATIONS 46 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 704 TO 1616
PROJECTED ANSWERS: 514 TO 1326

L9 46 SEA SSS SAM L8

=> s 19 sss full
FULL SEARCH INITIATED 18:01:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1129 TO ITERATE

100.0% PROCESSED 1129 ITERATIONS 891 ANSWERS
SEARCH TIME: 00.00.01

L10 891 SEA SSS FUL L8

=> s 18 sss full
FULL SEARCH INITIATED 18:01:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1129 TO ITERATE

100.0% PROCESSED 1129 ITERATIONS 891 ANSWERS

10/616031

SEARCH TIME: 00.00.01

L11 891 SEA SSS FUL L8

=> save l11

ENTER NAME OR (END) :ten616031/a

'TEN616031/A' IN USE

A single name cannot be used for two saved items at the same time. Enter "Y" if you wish to replace the current saved name with a new definition. Enter "N" if the current saved definition must be preserved. You may then reenter the SAVE command with a different saved name. Enter "DISPLAY SAVED" at an arrow prompt (=>) to see a list of your currently defined saved names.

REPLACE OLD DEFINITION? Y/(N):y

ANSWER SET L11 HAS BEEN SAVED AS 'TEN616031/A'

=> file caplus

COST IN U.S. DOLLARS

	SINCE FILE	TOTAL
	ENTRY	SESSION

FULL ESTIMATED COST

485.71	654.44
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE	TOTAL
	ENTRY	SESSION

CA SUBSCRIBER PRICE

0.00	-0.73
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FILE COVERS 1907 - 25 Jun 2005 VOL 143 ISS 1

FILE LAST UPDATED: 24 Jun 2005 (20050624/ED)

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=> s l11

L12 2 L11

=> d l12 1-2 bib abs fhitstr

L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:41225 CAPLUS

DN 140:111271

TI Preparation of pyrrolecarboxamides as HIV integrase inhibitors

IN Walker, Michael A.; Ma, Zhuping; Naidu, B. Narasimhulu; Sorenson, Margaret E.; Pendri, Annapurna; Banville, Jacques; Plamondon, Serge; Remillard, Roger

PA Bristol-Myers Squibb Company, USA

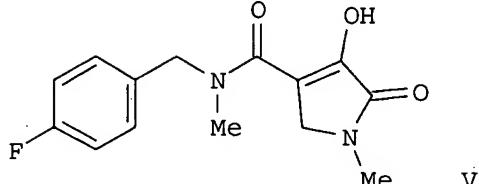
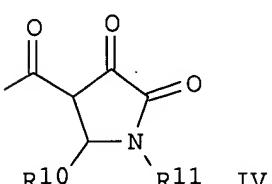
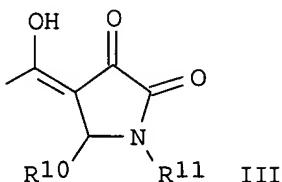
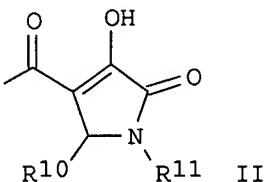
10/616031

SO PCT Int. Appl., 331 pp.
CODEN: PIXXD2

DT Patent
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004004657	A2	20040115	WO 2003-US21371	20030709
	WO 2004004657	A3	20041104		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2004110804	A1	20040610	US 2003-616031	20030709
PRAI	US 2002-394548P	P	20020709		
	US 2002-399248P	P	20020729		
OS	MARPAT 140:111271				
GI					



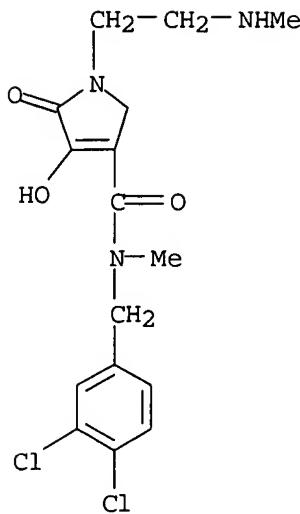
AB The title compds. R1CHR2NR3B1 [I; R1 = (un)substituted Ph, naphthyl, furyl, etc.; R2 = H, alkyl, (un)substituted aryl, alkylaryl; R3 = H, alkyl, alkylaryl, (un)substituted OH; B1 = II-IV (wherein R10 = H, alkyl, cycloalkyl, etc.; R11 = alkyl, cycloalkyl, aryl, etc.)] which inhibit HIV integrase, and are useful for treatment of AIDS or ARC, were prepared E.g., a multi-step synthesis of V which showed 99.9% inhibition of HIV integrase at 20 μ M, was given. Pharmaceutical composition comprising the compds. I is claimed.

IT 646042-18-4P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrrolecarboxamides as HIV integrase inhibitors)

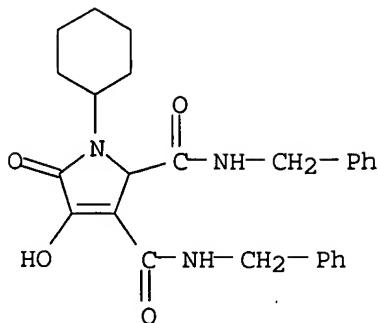
RN 646042-18-4 CAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[(3,4-dichlorophenyl)methyl]-2,5-dihydro-4-hydroxy-N-methyl-1-[2-(methylamino)ethyl]-5-oxo- (9CI) (CA INDEX NAME)



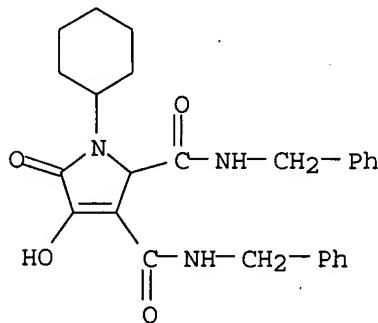
L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1968:114457 CAPLUS
 DN 68:114457
 TI 1-Carbamoyl- and 1-aminomethyl-1,4-dihydropyrrolo[3,4-b]indole derivatives. Indole formation by fragmentation of strain-barrier stabilized 2-aminoindoline derivatives
 AU Southwick, Philip L.; Vida, Julius A.; Fitzgerald, Berenice M.; Lee, Sung Ki
 CS Carnegie-Mellon Univ., Pittsburgh, PA, USA
 SO Journal of Organic Chemistry (1968), 33(5), 2051-6
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 GI For diagram(s), see printed CA Issue.
 AB 1-Substituted-4,5-dicarbethoxy-2,3-dioxopyrrolidines were prepared by addition of primary amines to di-Et maleate, followed by base-catalyzed condensation of the resulting N-substituted di-Et aspartates with Et oxalate. Base-catalyzed amide-ester interchange performed on the 1-cyclohexyl derivative with cyclohexylamine or benzylamine then afforded 1-cyclohexyl-4,5-bis(N-substituted carbamoyl)-2,3-dioxopyrrolidines (I). When treated with acids, I phenylhydrazones underwent the initial transformations of the Fischer indole synthesis to yield 3a-amino-1,8b-bis(N-substituted carbamoyl) - 2 - cyclohexyl - 1,3a,4,8b - tetrahydropyrrolo[3,4 - b]indol-3(2H)-ones (II), which failed to undergo the normal spontaneous NH₃ elimination, and therefore did not form the strained ring system of the corresponding indolenines. Instead, at elevated temps. under acidic or basic conditions II underwent a smooth fragmentation with elimination of both the 3a-amino and 8b-carbamoyl groups to yield 1-(N-substituted carbamoyl)-2 - cyclohexyl - 1,4 - dihydropyrrolo[3,4 - b]indol - 3(2H) - ones (III). LiAlH₄ reduction of III under appropriate conditions yielded 1-(N-substituted carbamoyl)- or 1-(N-substituted-aminomethyl)-1,4-dihydropyrrolo[3,4-b]indoles (IV). IV represent a new type of tryptamine analog. 11 references.
 IT 16206-08-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 16206-08-9 CAPLUS
 CN 3-Pyrroline-2,3-dicarboxamide, N,N'-dibenzyl-1-cyclohexyl-4-hydroxy-5-oxo-(8CI) (CA INDEX NAME)

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=> d 112 2 hitstr

L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
IT 16206-08-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16206-08-9 CAPLUS
CN 3-Pyrroline-2,3-dicarboxamide, N,N'-dibenzyl-1-cyclohexyl-4-hydroxy-5-oxo-
(8CI) (CA INDEX NAME)



=> file caold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

13.52 667.96

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SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent

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assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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L1 STRUCTURE UPLOADED
L2 2 S L1
L3 34 S L1 SSS FULL
 SAVE L3 TEN616031/A

FILE 'CAPLUS' ENTERED AT 17:55:18 ON 25 JUN 2005

L4 1 S L3

FILE 'REGISTRY' ENTERED AT 17:58:23 ON 25 JUN 2005

L5 STRUCTURE UPLOADED
L6 0 S L5
L7 0 S L5 SSS FULL
L8 STRUCTURE UPLOADED
L9 46 S L8
L10 891 S L9 SSS FULL
L11 891 S L8 SSS FULL
 SAVE L11 TEN616031/A

FILE 'CAPLUS' ENTERED AT 18:02:18 ON 25 JUN 2005

L12 2 S L11

FILE 'CAOLD' ENTERED AT 18:04:10 ON 25 JUN 2005

=> s l11
L13 0 L11

=> file chemcats

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FULL ESTIMATED COST	0.43	668.39
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.19

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L14 0 L11

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	ENTRY	SESSION
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FULL ESTIMATED COST	0.88	669.27
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CA SUBSCRIBER PRICE	ENTRY	SESSION
	0.00	-2.19

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